

Fermion Cluster Algorithms

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Cluster algorithms have been recently used to eliminate sign problems that plague Monte-Carlo methods in a variety of systems. In particular such algorithms can also be used to solve sign problems associated with the permutation of fermion world lines. This solution leads to the possibility of designing fermion cluster algorithms in certain cases. Using the example of free non-relativistic fermions we discuss the ideas underlying the algorithm.

1. INTRODUCTION

Fermions are quite difficult to deal with in Monte-Carlo methods. The main problem is the Pauli principle which introduces negative Boltzmann weights when fermions are treated physically as particles traveling in time. Until a few months ago the only known approach was to integrate them out and hope that the remaining problem is described by a positive Boltzmann weight. This approach has been successful in a few cases of physical interest like lattice QCD at zero chemical potential and zero vacuum angle. Unfortunately, even in these cases the Hybrid-Monte-Carlo methods slow down dramatically due to critical slowing down in the chiral limit [1].

Recently a new class of fermion algorithms have been discovered where the fermions are treated as physical particles traveling in time [2]. Such world line algorithms had been suggested in the past, however no solution to the fermion sign problem was found[3,4]. We have been able to solve this problem using cluster algorithms in a limited class of models. The progress is due to a better understanding of the relation between the topology of clusters and the effect of their flip on the fermion permutation sign. In certain cases, this knowledge can be used to completely eliminate the fermion sign problem and at the same time gain from the ability of cluster algorithms to beat critical slowing down. Thus, when successful these algorithms lead to the most ideal fermion algorithms discovered so far.

2. SIGN PROBLEM AND SOLUTION

The fermionic cluster algorithms that we have discovered are based on the cluster algorithm for a bosonic quantum spin-1/2 model. It is well known that a site with a fermion can be identified with a spin “up” state and an empty site with a spin “down” state up to sign factors that arise due to the Pauli principle. For every spin configuration the spin “up” states can be used to track fermion world lines which are closed in Euclidean time and describe a permutation of fermions. The sign of this permutation is exactly the same as the product of sign factors that arise from the Pauli principle. Hence it is always possible to absorb the physics of the Pauli principle into the sign of the Boltzmann weight of the spin configuration. Mathematically, the fermionic partition Z_f can be written as

$$Z_f = \sum_{[C]} \text{Sign}[C] W_b[C], \quad Z_b = \sum_{[C]} W_b[C], \quad (1)$$

where Z_b is the partition function of the quantum spin model written as a sum over configurations C , defined by a set C_i , $i = 1, 2, \dots, N_C$ of connected spin clusters, with a positive Boltzmann weight $W_b[C]$. In general the sign factor in Z_f is a product of the fermion permutation sign $\text{Sign}_f[C]$, discussed above and other local sign factors $\text{Sign}_b[C]$, that may be necessary to relate the fermionic and the bosonic models. Further, the existence of a cluster algorithm implies that the weight $W_b[C]$ remains the same if all the spins of any connected spin-cluster are flipped. On the other hand the 2^{N_C} degenerate configurations, obtained by flip-

*This work was supported in part by US department of energy grant DE-FG02-96ER40945.

ping the clusters, can have different sign factors $\text{Sign}[\mathcal{C}]$.

Although the above method of writing the fermionic model in terms of clusters of a bosonic model is well known, the freedom in choosing the bosonic weights $W_b[\mathcal{C}]$ and local bosonic sign factors $\text{Sign}_b[\mathcal{C}]$ had not been exploited until now. We have discovered that it is always possible to be clever in using this freedom so that the connected spin-clusters contribute independently to the sign of the configuration, i.e., the overall sign can always be written as $\text{Sign}[\mathcal{C}] = \prod_{i=1}^{N_C} \text{Sign}(\mathcal{C}_i)$, where $\text{Sign}(\mathcal{C}_i)$ is the sign associated with a connected cluster of spins. If $\text{Sign}[\mathcal{C}_i]$ changes when the spins are flipped the cluster is called a *meron*². Thus, meron clusters identify two spin configurations with the same weight but opposite signs and hence only non-meron clusters contribute to the partition function. It is always possible to include a Metropolis decision during the cluster formation process to suppress meron clusters in a controlled way. In certain models the spins within any connected cluster can always be flipped to a reference pattern $\mathcal{C}_i^{\text{ref}}$ such that $\text{Sign}[\mathcal{C}_i^{\text{ref}}] = 1$. In such cases the average of $\text{Sign}[\mathcal{C}]$ under all the 2^{N_C} flips of connected spin-clusters is 1 in the zero meron sector and this solves the sign problem completely.

3. MODELS AND ALGORITHMS

There are a variety of models that can be solved using the above ideas. Here we discuss how these ideas can be applied to solve free non-relativistic fermions on a d-dimensional hyper-cubic lattice described by the Hamiltonian,

$$H = \sum_{x,i} \left(n_x + n_{x+\hat{i}} - [c_x^\dagger c_{x+\hat{i}} + c_{x+\hat{i}}^\dagger c_x] \right), \quad (2)$$

where $n_x = c_x^\dagger c_x$ is the fermionic occupation number and c_x^\dagger and c_x are creation and annihilation operators. This model was originally considered in [3]. However, due to a wrong choice of $W_b[\mathcal{C}]$ and $\text{Sign}_b[\mathcal{C}]$, even this simple model appeared intractable numerically. Here we show how a different choice of these factors solves the

²This word was originally used in [5] to describe clusters with the same property in a classical $O(3)$ model.

problem completely. Following [3] we construct the partition function $Z_f = \text{Tr}[\exp(-\beta H)]$ by discretizing the Euclidean time axis into $2d \times M$ steps such that at a given time slice each spin interacts with only one neighboring spin. Thus, the Boltzmann weight of any configuration of fermion occupation numbers is a product of two-spin transfer matrix elements up to the global fermion permutation sign. Figure 1 illustrates a typical configuration in the path integral with the shaded regions representing the two spin interactions.

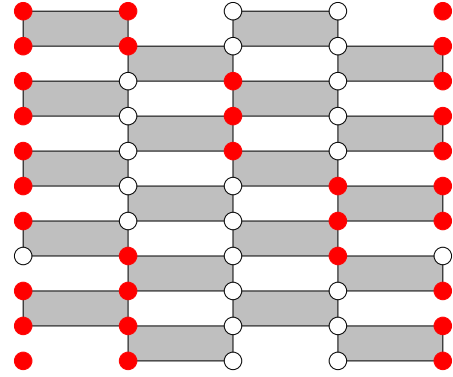


Figure 1. A typical spin configuration whose Boltzmann weight (up to an overall constant) is $e^{-3\epsilon e^{3\epsilon} [\cosh(\epsilon)]^{10} [\sinh(\epsilon)]^4}$ and the fermion permutation sign is -1 . Here $\epsilon = \beta/M$.

In order to construct the cluster algorithm we next introduce bond variables in addition to spin variables to describe connected spin-clusters and find transfer matrix elements for these new types of connected spin configurations such that the partition function remains the same. A given spin configuration can represent many spin-cluster configurations all of which have the same global fermion permutation sign. If we allow the transfer matrix elements of these new configurations to be negative there is a lot of freedom in choosing the weights and signs. Figure 2., illustrates a particular choice such that summing over the bond variables reproduces the weights of spin configurations. An interesting feature of the spin connection rules of figure 2 is that all spins in a connected cluster are of the same type. Further,

the negative sign associated with the cross bond configuration with all “up” spins is an extra local negative sign that can be absorbed into $\text{Sign}_b[\mathcal{C}]$, whereas the global fermion permutation sign is absorbed into the factor $\text{Sign}_f[\mathcal{C}]$. The model de-

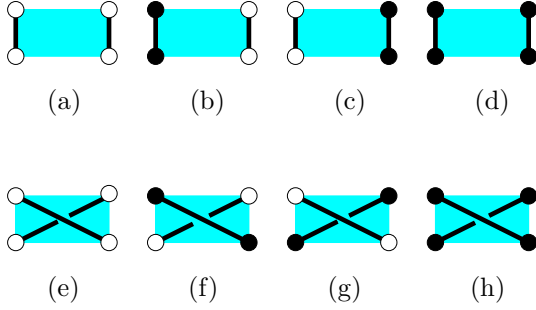


Figure 2. Transfer matrix elements of spin-cluster configurations. The weights of (a), (b), (c) and (d) are $\cosh(\epsilon)$, (e), (f) and (g) are $\sinh(\epsilon)$ and (h) is $-\sinh(\epsilon)$.

scribed by the magnitude of the weights of figure 2, is the spin-1/2 ferromagnetic Heisenberg model and can be updated using a cluster algorithm. Remarkably, $\text{Sign}[\mathcal{C}] = \text{Sign}_f[\mathcal{C}] \text{Sign}_b[\mathcal{C}]$ has all the desirable properties described in the previous section. The sign of a connected spin cluster is set to 1 if it is a cluster of “down” spins or if the temporal winding of the cluster is odd. Otherwise the sign of that cluster is -1 . Thus, clusters with an even temporal winding are merons.

In summary we have shown that clusters generated with the cluster algorithm of the ferromagnetic quantum spin-1/2 Heisenberg model, can also describe free non-relativistic fermions whose Hamiltonian is given in eq.(2), if we throw away clusters with an even temporal winding. In order to demonstrate the correctness of this observation we have calculated the two point fermion Greens function defined as

$$G(x, y; t) = \frac{1}{Z_f} \text{Tr} \left(e^{[-(\beta-t)H]} c_x e^{[-tH]} c_y^+ \right), \quad (3)$$

on a $4 \times 4 \times 4$ lattice at $\beta = 1$ and $M = 16$. Figure 3 shows this function in momentum space for $\vec{p} = (0, 0, 0)$ and $\vec{p} = (\pi, 0, 0)$. Evidently, the exact zero mode of H at zero momentum does

not lead to any complications, unlike conjugate gradient methods.

It is possible to extend the model to include short range repulsive interactions. In addition, the above ideas are also applicable in a variety of models with a rich phase structure. One such model has a finite temperature chiral phase transition and was studied extensively in [6]. The cluster algorithm of the anti-ferromagnetic Heisenberg model plays an important role there. Remarkably one can work directly in the chiral limit and no critical slowing down is observed.

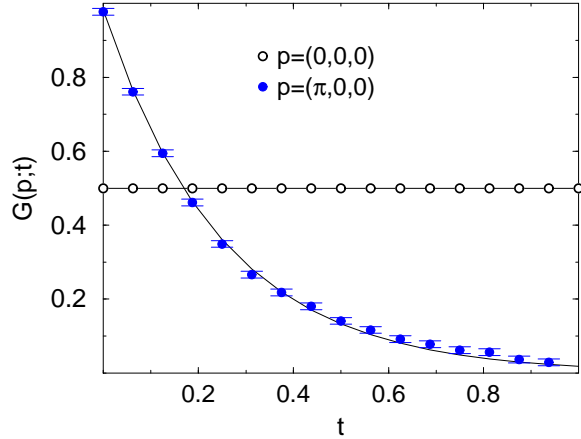


Figure 3. Two point correlation function in momentum space. The solid lines represent exact results.

All this shows that fermion cluster algorithms can provide a very elegant method to solve fermionic field theories numerically.

I wish to thank Uwe Wiese for his collaboration and many discussions at various stages of this work.

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